

Chemical Information:

Name: Valerenic acid
CAS No.: 3569-10-6
Tox21_ID No.: Tox21_200313
NTP_CID No.: 1389

Supplier: ChromaDex
Lot No.: 00022150-93A
MW: 234.33 g/mol

Date of Analysis: 13 May 2010

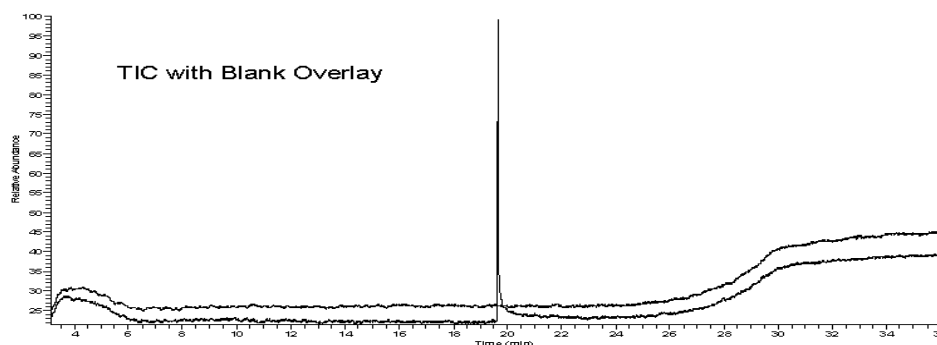
Purity and Identity Results:

Peak Identity	Retention Time (min)	Purity (% Total Area) ^a
Valerenic acid	19.66	100.00

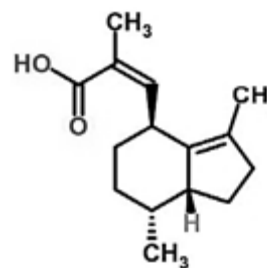
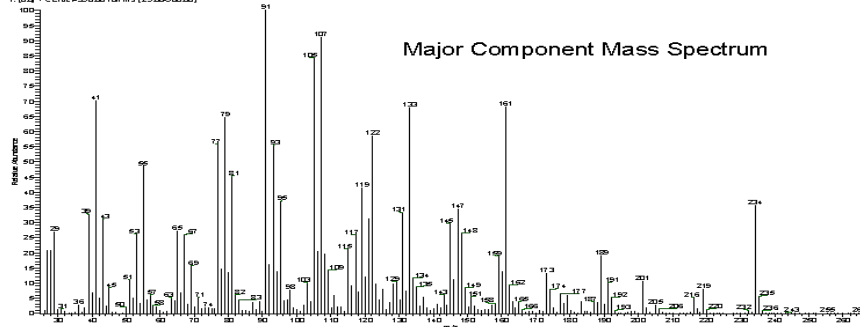
^a Peaks comprising $\geq 0.5\%$ of total area.

GC/MS Instrument Parameters:

Instrument / Ionization	Gas Chromatograph with Mass Spectrometer / Electron Impact
Solvent	Dichloromethane
Column	J&W Scientific HP-5MS, 30 m x 0.25 mm ID, 0.25- μ m film thickness
Carrier Gas	Helium at 1.0 mL/min
Oven Program	35°C, hold 2 min; ramp @ 10°C/min to 310°C, hold 7 min
Source Temperature	250°C
Auxiliary Temperature	250°C
Scan Range	25 – 500 amu
Injector Temperature	250°C
Injection Volume / Mode	1 μ L / Split (100:1)
Data Analysis Software	Xcalibur ver 1.2, and NIST Library ver 2.0f, build 10/08/2008



10112716 8 1963-1966 RT: 19.66-19.67 AM: 3 SE: 2 19.64-19.73 NL: 19785
T: 0.03 * C1818-350.00 FWHM: 25.03 s (0.00)


Mass Ion (C₁₂H₁₈O₂) = m/z 234

m/z	Fragment	m/z	Fragment
189	C ₁₄ H ₂₁	91	C ₇ H ₇
161	C ₁₁ H ₁₃ O	79	C ₆ H ₇
133	C ₁₀ H ₁₃	65	C ₅ H ₅
122	C ₉ H ₁₄	55	C ₄ H ₇
107	C ₈ H ₁₁	41	C ₃ H ₅